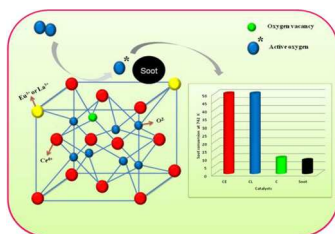


## CONTENTS

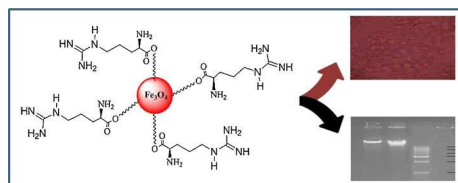
### Regular Articles



#### Tuning the structural and catalytic properties of ceria by doping with $\text{Zr}^{4+}$ , $\text{La}^{3+}$ and $\text{Eu}^{3+}$ cations

T Vinodkumar, D Naga Durgasri, Swamy Maloth and Benjaram M Reddy . . . . . 1145–1153

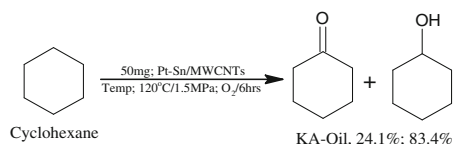
Preparation and activity of  $\text{La}^{3+}$ ,  $\text{Eu}^{3+}$ , and  $\text{Zr}^{4+}$  doped ceria-based materials are described. These materials are more active than pure ceria for soot oxidation. Among them, trivalent dopants effectively modified the catalytic properties of pure ceria.



#### Hydroxy, carboxylic and amino acid functionalized superparamagnetic iron oxide nanoparticles: Synthesis, characterization and *in vitro* anti-cancer studies

Dilaveez Rehana, Azees Khan Haleel and Aziz Kalilur Rahiman . . . . . 1155–1166

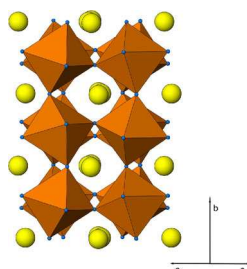
Superparamagnetic magnetite nanoparticles coated with different acids were synthesized and characterized. The cytotoxicity of nanoparticles was observed using MTT assay on adenocarcinoma (A549) cancer cells. Paclitaxel drug loaded, L-arginine coated nanoparticles showed highest cytotoxicity. DNA fragmentation on A549 cell line resulted in the breakdown of DNA molecules proving anti-cancer activity of the nanoparticles.



#### Efficient Aerobic Oxidation of Cyclohexane to KA Oil Catalyzed by Pt-Sn supported on MWCNTs

Mohammad Sadiq, Muhammad Ali, Rashid Iqbal, Khalid Saeed, Aimal Khan, Muhammad Naveed Umar and Haroon Ur Rashid . . . . . 1167–1172

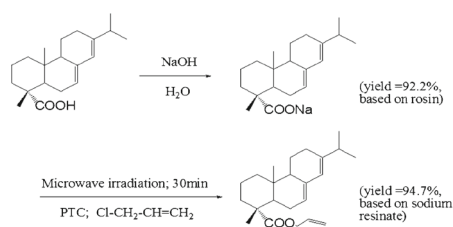
Pt-Sn/MWCNTs catalyst was efficiently used for the partial oxidation of cyclohexane into cyclohexanol and cyclohexanone in Parr type reactor, without any radical initiator or free radical scavenger.



#### Synthesis and crystal structure determination of $\text{YCo}_{1-x}\text{Fe}_x\text{O}_3$ ( $x = 0, 0.33, 0.5, 0.67$ and 1) perovskites

S Dimitrovska-lazova, S Aleksovska and P Tzvetkov . . . 1173–1181

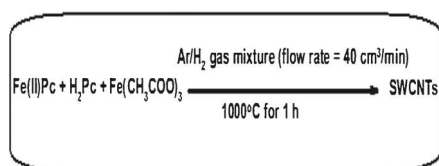
The perovskites  $\text{YCo}_{1-x}\text{Fe}_x\text{O}_3$  ( $0 \leq x \leq 1$ ) obtained by solution combustion method are isomorphous and crystallize in *Pnma* space group. The main reason for deviation from the ideal perovskite structure is tilting of the octahedra. The substitution of  $\text{Co}^{3+}$  with  $\text{Fe}^{3+}$  leads to a more distorted and tilted octahedron.



### Facile synthesis of allyl resinate monomer in an aqueous solution under microwave irradiation

Yanju Lu, Mixia Wang, Zhendong Zhao, Yuxiang Chen, Shichao Xu, Jing Wang and Liangwu Bi . . . . . 1183–1190

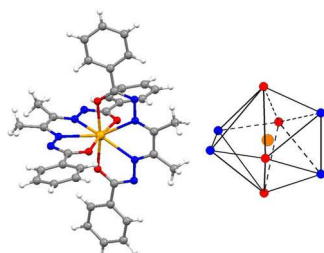
A facile method for production of allyl resinate monomer via a phase transfer reaction was developed. Microwave irradiation could significantly improve the formation of allyl resinate monomer. The replacement of solvents with water has potential to reduce the production cost of the monomers.



### Synthesis of single-walled carbon nanotubes by the pyrolysis of a compression activated iron(II) phthalocyanine/phthalocyanine metal-free derivative/ferric acetate mixture

Tawanda Mugadza, Edith Antunes and Tebello Nyokong . . . 1191–1199

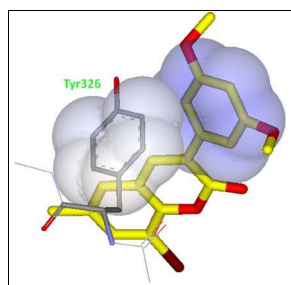
This paper reports on the synthesis of SWCNTs from an activated mixture of iron (II) phthalocyanine, its metal-free derivative and ferric acetate. Characterization of the synthesized SWCNTs was done using TEM, TGA, XRD and UV-vis, FTIR and Raman spectroscopies.



### Synthesis and characterization of dodecahedral cerium(IV) and gadolinium(III) complexes with a tetradentate Schiff Base

Tulika Ghosh and Samudranil Pal . . . . . 1201–1209

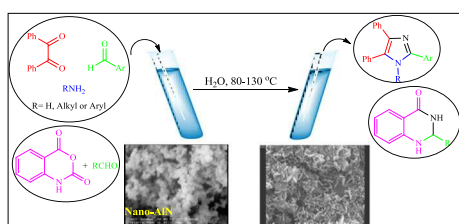
Two octacoordinated complexes [Ce(babh)<sub>2</sub>] and [Gd(babh)(Hbabh)] (H<sub>2</sub>babh = biacetyl bis(benzoylhydrazone)) are reported. They are characterized by microanalytical, crystallographic, spectroscopic and magnetic measurements. The meridional ONNO-donor ligands assemble a distorted dodecahedral N<sub>4</sub>O<sub>4</sub> coordination sphere in each complex. Self-assembly of the solvated complexes via intermolecular non-covalent interactions generates 1D ladder and 2D sheet structures.



### Quantum chemical analysis of potential anti-Parkinson agents

Nima Razzaghi-Asl, Sara Shahabipour, Ahmad Ebadi and Azam Bagheri . . . . . 1211–1220

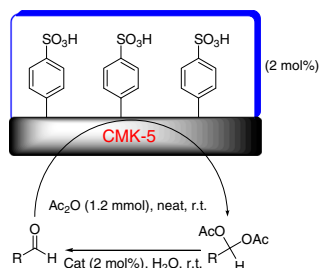
Binding mode of several 3-phenylcoumarin based MAO-B inhibitors were explored via molecular docking and analysis of intermolecular binding energy components. Structure activity relationship (SAR) studies indicated that coumarin ring may be a good substitution pattern for indan ring of Rasagiline in binding to the MAO-B active site.



### Green synthesis of tri/tetrasubstituted 1H-imidazoles and 2,3-dihydroquinazolin-4(1H)-ones using nano aluminium nitride as solid source of ammonia

Maryam Hajjami, Arash Ghorbani-Choghamarani, Zakieh Yousofvand and Masoomeh Norouzi . . . . . 1221–1228

An environmentally benign one-pot synthesis of tri/tetrasubstituted-1H-imidazoles and 2,3-dihydroquinazolin-4(1H)-ones using nano aluminium nitride as solid source of ammonia is reported.

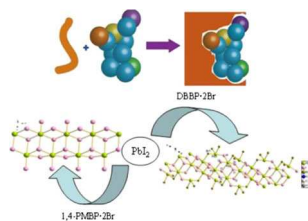


### Green procedures for the chemoselective synthesis of acylals and their cleavage promoted by recoverable sulfonic acid based nanoporous carbon (CMK-5- $\text{SO}_3\text{H}$ )

Daryoush Zareyee, Ehsan Mirzajanzadeh and

Mohammad Ali Khalilzadeh . . . . . 1229–1234

Recyclable nanoporous solid sulfonic acid (CMK-5- $\text{SO}_3\text{H}$ )-catalyzed synthesis of gem-diacetates from the reaction of aldehydes and acetic anhydride under solvent-free reaction conditions are reported. The catalyst was also found to be highly active for deprotection of resulting acylals in water.

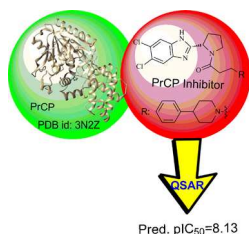


### Syntheses and characterization of two novel 1D Pb(II) Halide supramolecular polymers possessing incomplete Cubane subunit directed by $\pi$ -conjugated Dication templates

Chengjie Ma, Mei Liu, Wenli Zhang, Haijuan Du, Yao Li,

Chaohai Wang and Yunyin Niu . . . . . 1235–1242

We report two novel 1D iodoplumbate supramolecular polymers which contain incomplete cubane subunit based on  $\pi$ -conjugated dication templates. These compounds have been further characterized by IR, UV–Vis spectra, elemental analysis and thermostability tests.

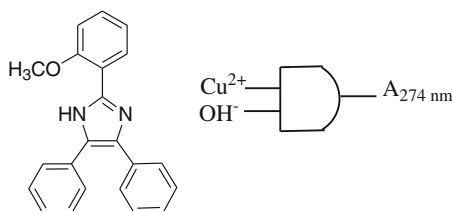


### QSAR study of prolylcarboxypeptidase inhibitors by genetic algorithm: Multiple linear regressions

Eslam Pourbasheer, Saadat Vahdani, Reza Aalizadeh, Alireza Banaei

and Mohammad Reza Ganjali. . . . . 1243–1251

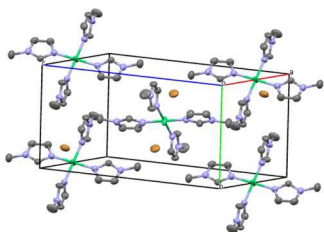
The predictive model using quantitative structure-activity relationships (QSAR) on benzimidazolepyrrolidiny amides as prolylcarboxypeptidase (PrCP) inhibitors was derived based on internally and externally validated robust GA-MLR model.



### An Imidazole based probe for relay recognition of $\text{Cu}^{2+}$ and $\text{OH}^-$ ions leading to AND logic gate

Navneet Kaur and Priya Alreja . . . . . 1253–1259

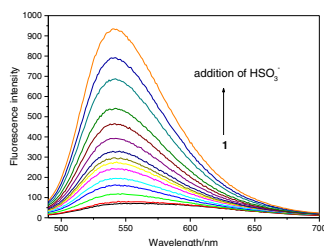
An imidazole based chemosensor **1** has been established as the molecular AND logic gate for relay recognition of  $\text{Cu}^{2+}$  and  $\text{OH}^-$  ions. The differential absorption changes observed with addition of  $\text{Cu}^{2+}$  and  $\text{OH}^-$  ions were used to mimic AND logic gate using  $A_{274 \text{ nm}}$  as output.



### Ionothermal synthesis and structural characterization of $[\text{Cu}(\text{C}_4\text{H}_6\text{N}_2)_4\text{Br}_2]$ and $[\text{Ni}(\text{C}_4\text{H}_6\text{N}_2)_4\text{Br}_2]$

Hong Wang, Bin Lu, Jingxiang Zhao and Qinghai Cai . . . 1261–1265

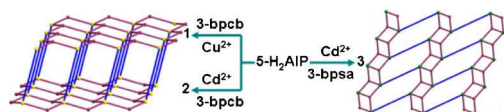
Two new complexes,  $\text{Cu}(\text{C}_4\text{H}_6\text{N}_2)_4\text{Br}_2$  and  $\text{Ni}(\text{C}_4\text{H}_6\text{N}_2)_4\text{Br}_2$  composed of complex cation formed by  $\text{Cu}^{2+}$  or  $\text{Ni}^{2+}$  coordinated by four N-methylimidazole ligands and bromide anions were ionothermally synthesized in an ionic liquid medium and characterized by X-ray single crystal diffraction, FT-IR, TGA and elemental analysis.



### A novel fluorescent turn-on probe for bisulfite based on NBD chromophore

Puhui Xie, Guangqin Gao, Wenjie Zhang, Guoyu Yang and Qiu Jin . . . . . 1267–1273

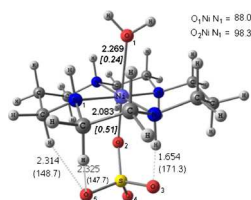
A novel fluorescent turn-on probe for bisulfite based on 7-nitrobenz-2-oxa-1,3-diazole (NBD) chromophore has been developed. The probe shows a selective, turn-on fluorescent response and ratiometric colorimetric response toward bisulfite in aqueous acetonitrile solutions.



### Three 2D copper(II)/cadmium(II) coordination polymers based on semi-rigid/flexible bis-pyridyl-bis-amide ligands and 5-aminoisophthalate: Syntheses, structures and properties

Hongyan Lin, Huizhe Lu, Mao Le, Jian Luan, Xiuli Wang and Guocheng Liu . . . . . 1275–1285

Three new copper(II)/cadmium(II) coordination polymers have been hydrothermally synthesized by self-assembly of 5-H<sub>2</sub>AIP, semi-rigid or flexible bis-pyridyl-bis-amide ligands and copper chloride or cadmium nitrate. The electrochemical behavior, the fluorescent and photocatalytic properties of the compounds have been investigated.

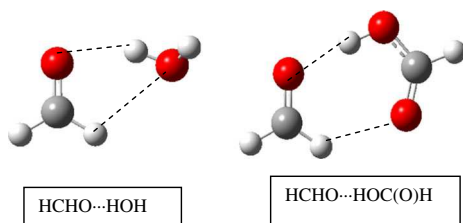


[NiL<sub>1</sub>(SO<sub>4</sub>)(H<sub>2</sub>O)]<sup>+</sup>

### Kinetic measurements and quantum chemical calculations on low spin Ni(II)/(III) macrocyclic complexes in aqueous and sulphato medium

Anuradha Sankaran, E J Padma Malar and Venkatapuram Ramanujam Vijayaraghavan . . . . . 1287–1298

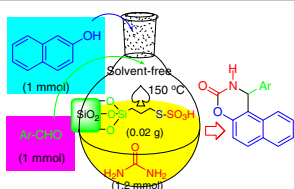
Complementary kinetic study and quantum chemical calculations describe the bonding in low-spin aqua and sulfato Ni(II) and Ni(III) macrocyclic complexes. Quantum chemical calculations demonstrate that the electronic and structural factors involving the macrocyclic ligand cause different modes of bonding between axial water and Ni(III) ion.



### Theoretical Characterization of Hydrogen Bonding Interactions between RCHO (R = H, CN, CF<sub>3</sub>, OCH<sub>3</sub>, NH<sub>2</sub>) and HOR' (R' = H, Cl, CH<sub>3</sub>, NH<sub>2</sub>, C(O)H, C<sub>6</sub>H<sub>5</sub>)

Damanjit Kaur and Rajinder Kaur . . . . . 1299–1313

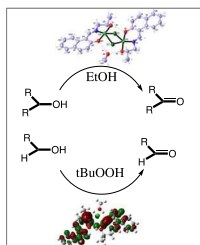
Theoretical calculations were carried out on the RCHO...HOR' (R = H, CN, CF<sub>3</sub>, OCH<sub>3</sub>, NH<sub>2</sub>; R' = H, Cl, CH<sub>3</sub>, NH<sub>2</sub>, C(O)H, C<sub>6</sub>H<sub>5</sub>) hydrogen bonded complexes. The role of substituents on hydrogen donor and acceptor ability has been explored on the basis of analysis of geometrical data, proton affinities, NBO, AIM, SAPT, MESP and stabilization energies.



### Synthesis of naphthoxazinone derivatives using silica-bonded S-sulfonic acid as catalyst under solvent-free conditions

Khodabakhsh Niknam and Parisa Abolpour . . . . . 1315–1320

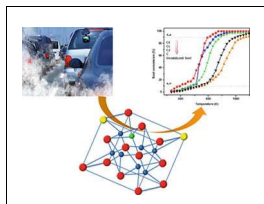
Silica-bonded S-sulfonic acid was employed as solid acid catalyst for the synthesis of naphthoxazinones under solvent-free conditions.



**A novel dinuclear schiff base copper complex as an efficient and cost effective catalyst for oxidation of alcohol: Synthesis, crystal structure and theoretical studies**

Atena Naeimi, Samira Saeednia, Mehdi Yoosefian, Hadi Amiri Rudbari and Viviana Mollica Nardo . . . . . 1321–1328

A novel  $[(HL)Cu(\mu_2-Cl)_2Cu(HL)] \cdot 1.5CH_3OH$  complex was used as an efficient catalyst for the oxidation of alcohols. It was synthesized, using (E)-1-(((2-hydroxypropyl)imino)methyl)naphthalen-2-ol as a monoanionic and tridentate Schiff base ligand, and characterized by IR and UV-Visible spectroscopy and single-crystal X-ray analysis. The geometry of the complex was optimized using the B3LYP level of theory.



*Cover picture:* Tuning properties of ceria for soot oxidation. For details, see the paper by T Vinodkumar *et al.* (pp. 1145–1153)